

Weak itinerant ferromagnetism in YCo_9Si_4

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Abstract

Weak itinerant ferromagnetism in YCo_9Si_4 below about 25 K is studied by means of magnetisation, specific heat, and resistivity measurements. Single crystal X-ray Rietveld refinements at room temperature reveal a fully ordered distribution of Y, Co and Si atoms within the tetragonal space group $I4/mcm$ isostructural with LaCo_9Si_4 . The latter exhibits itinerant electron metamagnetism with an induced moment of about $1 \mu_B/\text{f.u.}$ above 6 T, whereas YCo_9Si_4 exhibits a spontaneous magnetisation $M_0 \simeq 12 \text{ Am}^2/\text{kg}$ at 2 K which corresponds to an ordered moment of about $1.6 \mu_B/\text{f.u.}$ indicating weak itinerant ferromagnetism.

Key words:

YCo_9Si_4 , itinerant magnetism, specific heat

Recent interest on weak itinerant ferromagnetism e.g. in ZrZn_2 [1] in the context with quantum critical phenomena motivated the search for new materials showing weak itinerant ferromagnetism or being close to a ferromagnetic (FM) instability. An interesting system in this respect is the solid solution $\text{LaCo}_{13-x}\text{Si}_x$ where ferromagnetism vanishes near the stoichiometric composition LaCo_9Si_4 [2] where full translational symmetry (space group $I4/mcm$) is confirmed by single crystal X-ray diffractometry [3]. LaCo_9Si_4 is a strongly exchange enhanced Pauli paramagnet and exhibits an itinerant electron metamagnetic phase transition at about 3.5 T for $H \parallel c$ and 6 T for $H \perp c$, which is the lowest value ever found for rare earth intermetallic compounds [3]. In this paper, we report on low temperature measurements on the isostructural and isoelec-

tronic compound YCo_9Si_4 which was initially reported in Refs. [4,5] to be FM with $T_C \simeq 848 \text{ K}$.

Polycrystalline samples of YCo_9Si_4 were synthesized by induction melting of pure elements (Y 3N, Co 4.5N, Si 6N) under protective argon atmosphere and subsequent annealing at 1050°C for one week. The phase purity and composition has been verified by means of electron microprobe analysis. The crystal structure was determined by means of single crystal X-ray diffraction ($R_{F2} = 2\%$) revealing a fully ordered distribution of Y, Co and Si atoms with the LaFe_9Si_4 -type [6] with a single rare earth site, three cobalt sites and again a single Si site. The lattice parameters are $a = 7.754(1) \text{ \AA}$ and $c = 11.487(1) \text{ \AA}$ at room temperature (see Ref. [3] for experimental details). Crystallographic order is also corroborated by a reasonably low residual resistivity $\rho_0 = 7 \mu\Omega\text{cm}$ (see below).

Temperature and field dependent magnetisation measurements $M(T, H)$ on YCo_9Si_4 depicted in Fig. 1 as an Arrott plot M^2 versus H/M reveal weak ferromagnetism below about 25 K with an extrapolated spontaneous magnetisation $M_0 \simeq 12 \text{ Am}^2/\text{kg}$ at 2 K (see the dashed line in Fig. 1) corresponding to

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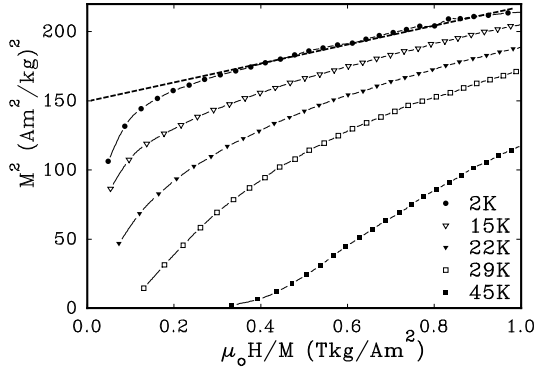


Fig. 1. Arrott plot M^2 vs. H/M of isothermal magnetization data of YCo_9Si_4 .

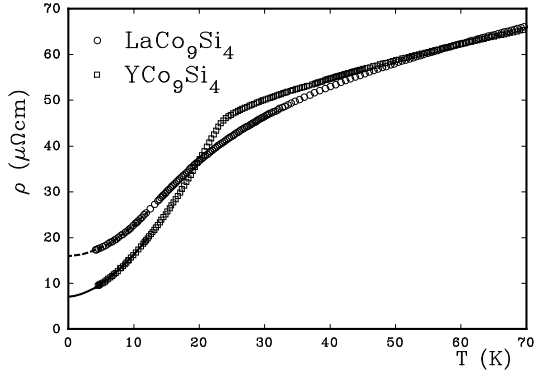


Fig. 2. Temperature dependent resistivity $\rho(T)$ of YCo_9Si_4 and LaCo_9Si_4 ; dashed and solid lines are fits, see text.

$1.6 \mu_B/\text{f.u.}$ and a longitudinal susceptibility in the FM regime, $\chi_0 \sim 0.25 \text{ Am}^2/\text{kgT}$, determined from the $\mu_0 H/M$ axis intercept of the dashed line extrapolation in Fig. 1. The Curie-temperature T_C is around 25 K in reasonable agreement with specific heat and transport anomalies (see below).

The temperature dependent resistivity $\rho(T)$ of YCo_9Si_4 shown in Fig. 2 reveals a significant change of slope around about 25 K which is associated with the onset of ferromagnetism. Below about 15 K, in the FM state, $\rho(T)$ is well described by a power law behavior $\rho(T) = \rho_0 + AT^\alpha$ (see the solid line in Fig. 2) with $\rho_0 = 7 \mu\Omega\text{cm}$, $A = 0.176 \mu\Omega\text{cm}/\text{K}^{-\alpha}$ and $\alpha = 1.72$. The corresponding fit for nearly ferromagnetic LaCo_9Si_4 (dashed line in Fig. 2) yields $\rho_0 = 16 \mu\Omega\text{cm}$, $A = 0.085 \mu\Omega\text{cm}/\text{K}^{-\alpha}$ and $\alpha = 1.9$ indicating a spin fluctuation (Fermi liquid) regime for the latter compound.

The specific heat of YCo_9Si_4 and (for comparison) LaCo_9Si_4 is shown in Fig. 3 as C/T vs. T revealing for both compounds a relatively large electronic Sommerfeld value γ close to $200 \text{ mJ}/\text{mol K}^2$ and in the case of YCo_9Si_4 a small somewhat broadened anomaly associated with the second order phase transition towards

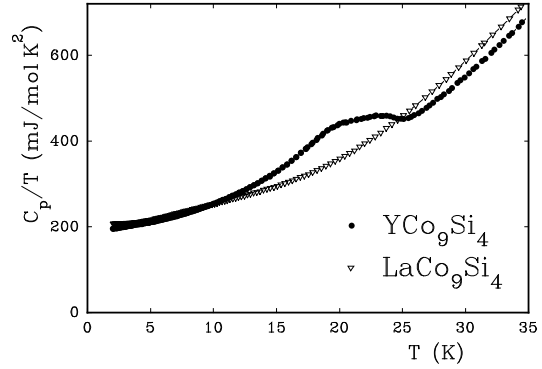


Fig. 3. Temperature dependent specific heat as C/T vs. T of YCo_9Si_4 and LaCo_9Si_4 .

weak itinerant ferromagnetism with a jump $\Delta C/T$ of the order of $100 \text{ mJ}/\text{mol K}^2$ in approximate agreement with the Stoner-Wohlfarth model (see e.g. Ref. [7]) yielding $\Delta C/T_C = M_0^2/\chi_0 T_C^2 \sim 70 \text{ mJ}/\text{mol K}^2$. In the case of exchange enhanced Pauli paramagnetic LaCo_9Si_4 the value of $\gamma \simeq 200 \text{ mJ}/\text{mol K}^2$ can be compared with the density of states obtained from *ab-initio* electronic structure calculations, $N(E_F) \sim 19 \text{ states}/\text{eV f.u.}$, revealing a spin-fluctuation mass enhancement $\lambda_{spin} \sim 3.3$ [3].

For YCo_9Si_4 band calculations have been performed in the same manner as described in Ref. [3] for LaCo_9Si_4 yielding practically the same picture with respect to the Co *d*-bands as for LaCo_9Si_4 and within the numerical accuracy the same density of states at the Fermi level. The spin-fluctuation mass enhancement λ_{spin} is thus very similar in YCo_9Si_4 and LaCo_9Si_4 . Band calculations at the experimental lattice constant yield a FM ground state for both compounds, which is experimentally confirmed only for YCo_9Si_4 while LaCo_9Si_4 shows a paramagnetic ground state and metamagnetism. In analogy to the conclusions drawn for LaCo_9Si_4 we expect also for YCo_9Si_4 in the FM state the largest moments of about $0.3\text{--}0.4 \mu_B/\text{Co}$ to be at the $16k$ Co-sites and significantly smaller moments at the $4d$ and $16l$ Co-sites.

References

- [1] C. Pfleiderer *et al.*, Nature (London) **412** (2001) 58.
- [2] M. El-Hagary *et al.*, J. Alloys Compounds **367** (2004) 239.
- [3] H. Michor *et al.*, Phys.Rev. B **69** (2004) 081404(R).
- [4] R.V. Skolozdra *et al.*, J. Alloys Compounds **296** (2000) 272.
- [5] Yu. Gorelenko *et al.*, Visnyk of the Lviv University, Series Chemical **43** (2003) 62.
- [6] W.H. Tang *et al.*, J. Appl. Phys. **76** (1994) 4095.
- [7] P. Mohn and G. Hilscher, Phys.Rev. B **40** (1989) 9126.